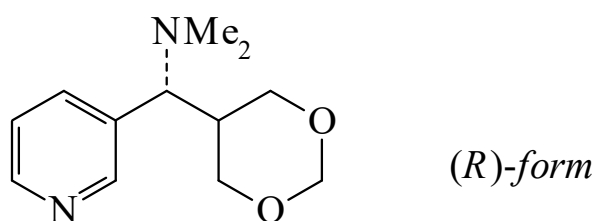




>>Entry Name: Doxpicomine, INN

Synonym(s): α -1,3-Dioxan-5-yl-*N,N*-dimethyl-3-pyridinemethanamine, 9CI. 3-[(Dimethylamino)(1,3-dioxan-5-yl)methyl]pyridine. Doxpicodin. Doxpizodine



Type of Compound Code(s): XA0650

Molecular Formula: C₁₂H₁₈N₂O₂

Molecular Weight: 222.286

Accurate Mass: 222.136828

Percentage Composition: C 64.84%; H 8.16%; N 12.60%; O 14.40%

General Statement: Strictly, the name Doxpicomine refers to the (*R*)-form

Use/Importance: Analgesic

Calculated Log P Data: Log P −0.96 (calc)

>>Variant: (*R*)-form

CAS Registry Number: 62904-71-6

Molecular Formula: C₁₂H₁₈N₂O₂

Molecular Weight: 222.286

Accurate Mass: 222.136828

Percentage Composition: C 64.84%; H 8.16%; N 12.60%; O 14.40%

>>Derivative: Hydrochloride

Synonym(s): Doxpicomine hydrochloride, USAN. LY 108380

CAS Registry Number: 69494-04-8

Use/Importance: Analgesic

Physical Description: Cryst. (EtOH)

Melting Point: Mp 234-236°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -17$ (c, 1 in MeOH)

Hazard & Toxicity: LD₅₀ (mus, scu) 1420 mg/kg

>>Variant: (±)-form

Molecular Formula: C₁₂H₁₈N₂O₂

Molecular Weight: 222.286

Accurate Mass: 222.136828

Percentage Composition: C 64.84%; H 8.16%; N 12.60%; O 14.40%

>>Derivative: Hydrochloride (1:2)

Melting Point: Mp 196-197°

References:

Booher, R.N. *et al.*, *J. Med. Chem.*, 1977, **20**, 885, (*pharmacol, synth, resoln*)

Rubin, A. *et al.*, *Drug Metab. Dispos.*, 1979, **7**, 149, (*metab*)

Wang, R.I.H. *et al.*, *Clin. Pharmacol. Ther. (St. Louis)*, 1981, **29**, 771, (*pharmacol*)

Martindale, *The Extra Pharmacopoeia*, 28th/29th edn., *Pharmaceutical Press*, 1982, 12679

Farkas, E. *et al.*, *J.O.C.*, 1985, **50**, 1110, (*synth*)